



# Full wwPDB NMR Structure Validation Report ⓘ

Feb 12, 2017 – 06:13 pm GMT

PDB ID : 1H8M  
Title : SOLUTION STRUCTURE OF YKT6  
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Deposited on : 2001-02-10

This is a Full wwPDB NMR Structure Validation Report for a publicly released PDB entry.

We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)

A user guide is available at

<http://wwpdb.org/validation/2016/NMRValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

Cyrange	:	Kirchner and Güntert (2011)
NmrClust	:	Kelley et al. (1996)
MolProbity	:	4.02b-467
Percentile statistics	:	20161228.v01 (using entries in the PDB archive December 28th 2016)
RCI	:	v_1n_11_5_13_A (Berjanski et al., 2005)
PANAV	:	Wang et al. (2010)
ShiftChecker	:	trunk28760
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	recalc28949

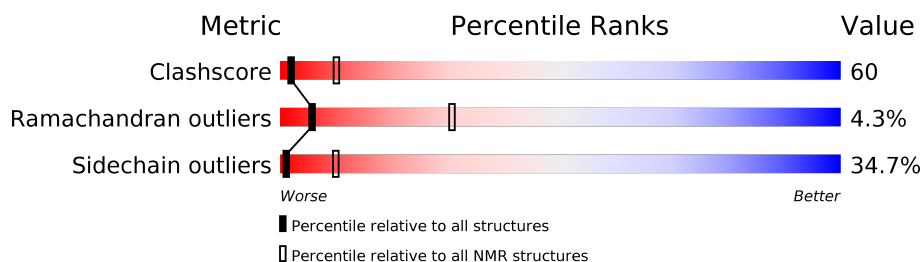
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*SOLUTION NMR*

The overall completeness of chemical shifts assignment was not calculated.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	NMR archive (#Entries)
Clashscore	125131	11601
Ramachandran outliers	121729	10391
Sidechain outliers	121581	10367

The table below summarises the geometric issues observed across the polymeric chains and their fit to the experimental data. The red, orange, yellow and green segments indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. A cyan segment indicates the fraction of residues that are not part of the well-defined cores, and a grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$

Mol	Chain	Length	Quality of chain
1	A	140	<div> <div style="width: 40%; background-color: green;"></div> <div style="width: 40%; background-color: yellow;"></div> <div style="width: 19%; background-color: orange;"></div> <div style="width: 1%; background-color: red;"></div> <div style="width: 0%; background-color: cyan;"></div> <div style="width: 0%; background-color: grey;"></div> </div> <div>40% 40% 19% .</div>

## 2 Ensemble composition and analysis ⓘ

This entry contains 1 models. Identification of well-defined residues and clustering analysis are not possible.

### 3 Entry composition

There is only 1 type of molecule in this entry. The entry contains 2201 atoms, of which 1084 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called SYNAPTOBREVIN HOMOLOG 1.

Mol	Chain	Residues	Atoms						Trace
1	A	140	Total	C	H	N	O	S	0
			2201	709	1084	184	220	4	

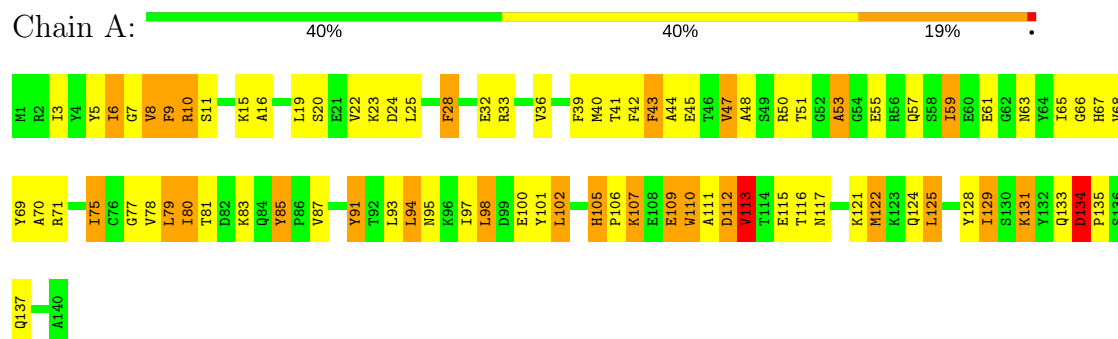
There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	55	GLU	GLN	CONFLICT	UNP P36015
A	84	GLN	GLU	CONFLICT	UNP P36015

## 4 Residue-property plots [i](#)

These plots are provided for all protein, RNA and DNA chains in the entry. The first graphic is the same as shown in the summary in section 1 of this report. The second graphic shows the sequence where residues are colour-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. Stretches of 2 or more consecutive residues without any outliers are shown as green connectors. Residues which are classified as ill-defined in the NMR ensemble, are shown in cyan with an underline colour-coded according to the previous scheme. Residues which were present in the experimental sample, but not modelled in the final structure are shown in grey.

### • Molecule 1: SYNAPTOBREVIN HOMOLOG 1



## 5 Refinement protocol and experimental data overview

Of the ? calculated structures, 1 were deposited, based on the following criterion: ?.

The following table shows the software used for structure solution, optimisation and refinement.

Software name
.014 DEG DIHEDRALS 29.969 DEG 0.887 DEG ENOE -30.74 40.95 ECDIH 3.28 0.40 EBOND 14.68 1.25

No chemical shift data was provided. No validations of the models with respect to experimental NMR restraints is performed at this time.

## 6 Model quality

### 6.1 Standard geometry

There are no covalent bond-length or bond-angle outliers.

There are no bond-length outliers.

There are no bond-angle outliers.

There are no chirality outliers.

There are no planarity outliers.

### 6.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in each chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes averaged over the ensemble.

Mol	Chain	Non-H	H(model)	H(added)	Clashes
1	A	1117	1084	1082	132
All	All	1117	1084	1082	132

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 60.

All clashes are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Clash(Å)	Distance(Å)
1:A:68:VAL:HG22	1:A:78:VAL:HG22	1.01	1.29
1:A:3:ILE:HG22	1:A:133:GLN:HA	0.91	1.38
1:A:44:ALA:HB2	1:A:80:ILE:HD11	0.85	1.47
1:A:110:TRP:HB2	1:A:113:VAL:HG22	0.82	1.51
1:A:47:VAL:HB	1:A:68:VAL:HG21	0.80	1.54
1:A:68:VAL:CG2	1:A:78:VAL:HG22	0.80	2.06
1:A:51:THR:OG1	1:A:68:VAL:HG11	0.77	1.77
1:A:3:ILE:HD11	1:A:6:ILE:HG13	0.76	1.57
1:A:79:LEU:HD12	1:A:94:LEU:HD23	0.75	1.58
1:A:79:LEU:HD11	1:A:93:LEU:HB3	0.74	1.59
1:A:6:ILE:HD12	1:A:129:ILE:HB	0.72	1.61
1:A:81:THR:HG21	1:A:85:TYR:CD1	0.70	2.21
1:A:43:PHE:O	1:A:47:VAL:HG22	0.70	1.87
1:A:6:ILE:HD11	1:A:93:LEU:HD13	0.68	1.65
1:A:47:VAL:HG13	1:A:59:ILE:CD1	0.67	2.19

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Atom-1	Atom-2	Clash(Å)	Distance(Å)
1:A:69:TYR:OH	1:A:87:VAL:HG12	0.66	1.90
1:A:32:GLU:O	1:A:36:VAL:HG23	0.65	1.92
1:A:47:VAL:HB	1:A:68:VAL:CG2	0.64	2.22
1:A:107:LYS:HA	1:A:110:TRP:CZ2	0.64	2.27
1:A:134:ASP:CB	1:A:135:PRO:HD2	0.64	2.23
1:A:94:LEU:HA	1:A:97:ILE:HG22	0.63	1.71
1:A:6:ILE:HB	1:A:129:ILE:HG13	0.63	1.71
1:A:94:LEU:HA	1:A:97:ILE:CG2	0.62	2.24
1:A:67:HIS:CE1	1:A:87:VAL:HG22	0.62	2.29
1:A:25:LEU:HD13	1:A:33:ARG:HB2	0.61	1.71
1:A:8:VAL:HB	1:A:19:LEU:HB3	0.60	1.73
1:A:105:HIS:CD2	1:A:105:HIS:N	0.59	2.70
1:A:66:GLY:HA2	1:A:80:ILE:CG2	0.59	2.27
1:A:59:ILE:HG13	1:A:66:GLY:HA3	0.59	1.75
1:A:9:PHE:CZ	1:A:44:ALA:HB1	0.59	2.33
1:A:134:ASP:HB3	1:A:135:PRO:HD2	0.58	1.74
1:A:100:GLU:HB3	1:A:122:MET:HE3	0.58	1.75
1:A:6:ILE:HD11	1:A:93:LEU:CD1	0.57	2.28
1:A:110:TRP:CB	1:A:113:VAL:HG22	0.57	2.25
1:A:6:ILE:HD11	1:A:79:LEU:HD21	0.57	1.77
1:A:111:ALA:O	1:A:112:ASP:HB2	0.57	2.00
1:A:6:ILE:HD12	1:A:129:ILE:CB	0.55	2.32
1:A:97:ILE:HG23	1:A:98:LEU:N	0.55	2.16
1:A:9:PHE:CE1	1:A:78:VAL:HB	0.55	2.36
1:A:7:GLY:HA2	1:A:125:LEU:CD1	0.55	2.32
1:A:47:VAL:HA	1:A:50:ARG:CG	0.55	2.32
1:A:6:ILE:HG22	1:A:22:VAL:CG1	0.55	2.32
1:A:3:ILE:HG22	1:A:133:GLN:CA	0.54	2.25
1:A:8:VAL:HG23	1:A:20:SER:OG	0.54	2.03
1:A:5:TYR:CD2	1:A:40:MET:HB3	0.54	2.38
1:A:8:VAL:C	1:A:9:PHE:CD1	0.54	2.81
1:A:75:ILE:HG21	1:A:110:TRP:CE3	0.53	2.38
1:A:44:ALA:O	1:A:47:VAL:HG23	0.53	2.03
1:A:69:TYR:HB2	1:A:94:LEU:HD12	0.53	1.81
1:A:22:VAL:CG1	1:A:129:ILE:HG21	0.52	2.34
1:A:3:ILE:HD11	1:A:6:ILE:CG1	0.52	2.30
1:A:112:ASP:C	1:A:113:VAL:HG23	0.52	2.23
1:A:6:ILE:CD1	1:A:129:ILE:HB	0.52	2.34
1:A:97:ILE:CG2	1:A:98:LEU:N	0.52	2.72
1:A:9:PHE:CD1	1:A:9:PHE:N	0.52	2.77
1:A:122:MET:HB2	1:A:125:LEU:HD22	0.51	1.82
1:A:9:PHE:CZ	1:A:44:ALA:CB	0.51	2.94

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Atom-1	Atom-2	Clash(Å)	Distance(Å)
1:A:65:ILE:CG2	1:A:66:GLY:N	0.51	2.74
1:A:19:LEU:CD2	1:A:75:ILE:HG13	0.50	2.36
1:A:66:GLY:CA	1:A:80:ILE:HG23	0.50	2.36
1:A:94:LEU:CA	1:A:97:ILE:HG22	0.50	2.35
1:A:75:ILE:CG2	1:A:110:TRP:CE3	0.50	2.95
1:A:47:VAL:HG13	1:A:59:ILE:HD13	0.50	1.83
1:A:53:ALA:HA	1:A:70:ALA:HB1	0.50	1.83
1:A:57:GLN:O	1:A:68:VAL:HB	0.49	2.07
1:A:94:LEU:HD22	1:A:97:ILE:HG21	0.49	1.83
1:A:19:LEU:HD21	1:A:101:TYR:CZ	0.49	2.43
1:A:28:PHE:CE2	1:A:40:MET:CE	0.49	2.96
1:A:47:VAL:CG1	1:A:59:ILE:CD1	0.48	2.92
1:A:6:ILE:HB	1:A:129:ILE:CG1	0.48	2.39
1:A:66:GLY:HA2	1:A:80:ILE:HG23	0.48	1.84
1:A:69:TYR:HB2	1:A:94:LEU:CG	0.47	2.39
1:A:9:PHE:HB2	1:A:48:ALA:CB	0.47	2.39
1:A:47:VAL:CB	1:A:68:VAL:HG21	0.47	2.34
1:A:8:VAL:HG13	1:A:77:GLY:CA	0.47	2.38
1:A:6:ILE:CG2	1:A:7:GLY:N	0.47	2.77
1:A:59:ILE:HG13	1:A:66:GLY:CA	0.47	2.38
1:A:66:GLY:CA	1:A:80:ILE:CG2	0.47	2.92
1:A:6:ILE:CD1	1:A:93:LEU:CD1	0.47	2.92
1:A:47:VAL:HA	1:A:50:ARG:HG3	0.47	1.87
1:A:25:LEU:HA	1:A:28:PHE:CD2	0.46	2.46
1:A:44:ALA:HA	1:A:78:VAL:HG11	0.46	1.87
1:A:6:ILE:CB	1:A:129:ILE:HG13	0.46	2.40
1:A:65:ILE:HG21	1:A:67:HIS:CE1	0.46	2.45
1:A:128:TYR:HA	1:A:131:LYS:HD3	0.46	1.88
1:A:134:ASP:CB	1:A:135:PRO:CD	0.46	2.94
1:A:6:ILE:CB	1:A:129:ILE:HB	0.46	2.41
1:A:69:TYR:HB2	1:A:94:LEU:CD1	0.46	2.41
1:A:97:ILE:CD1	1:A:125:LEU:HB2	0.46	2.41
1:A:8:VAL:HA	1:A:77:GLY:HA2	0.46	1.87
1:A:28:PHE:CE2	1:A:40:MET:HE1	0.45	2.46
1:A:79:LEU:CD1	1:A:93:LEU:HB3	0.45	2.37
1:A:112:ASP:O	1:A:113:VAL:HG23	0.45	2.11
1:A:10:ARG:HB2	1:A:75:ILE:HB	0.45	1.89
1:A:7:GLY:HA2	1:A:125:LEU:HD11	0.45	1.86
1:A:3:ILE:HG13	1:A:81:THR:HB	0.45	1.89
1:A:94:LEU:HD13	1:A:97:ILE:CG2	0.45	2.42
1:A:19:LEU:HD21	1:A:101:TYR:CE2	0.44	2.47
1:A:79:LEU:HD12	1:A:94:LEU:CD2	0.44	2.37

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Atom-1	Atom-2	Clash(Å)	Distance(Å)
1:A:5:TYR:CG	1:A:40:MET:HB3	0.44	2.47
1:A:105:HIS:HB2	1:A:109:GLU:HG2	0.44	1.89
1:A:94:LEU:C	1:A:97:ILE:HG22	0.44	2.32
1:A:111:ALA:O	1:A:112:ASP:CB	0.43	2.66
1:A:98:LEU:O	1:A:102:LEU:HG	0.43	2.13
1:A:57:GLN:O	1:A:68:VAL:N	0.43	2.51
1:A:6:ILE:O	1:A:22:VAL:HG12	0.43	2.14
1:A:112:ASP:C	1:A:113:VAL:CG2	0.43	2.86
1:A:97:ILE:HG13	1:A:125:LEU:CB	0.43	2.44
1:A:6:ILE:HB	1:A:129:ILE:CB	0.42	2.44
1:A:79:LEU:CD1	1:A:94:LEU:HD23	0.42	2.39
1:A:9:PHE:O	1:A:48:ALA:HB1	0.42	2.14
1:A:16:ALA:CB	1:A:48:ALA:HB3	0.42	2.43
1:A:66:GLY:HA2	1:A:80:ILE:HA	0.42	1.90
1:A:5:TYR:CB	1:A:40:MET:HB3	0.42	2.45
1:A:5:TYR:CD1	1:A:6:ILE:N	0.42	2.87
1:A:91:TYR:O	1:A:95:ASN:HB2	0.41	2.15
1:A:22:VAL:HG11	1:A:129:ILE:HG21	0.41	1.91
1:A:3:ILE:CD1	1:A:6:ILE:HG13	0.41	2.36
1:A:102:LEU:HD22	1:A:110:TRP:CZ2	0.41	2.51
1:A:6:ILE:HG22	1:A:125:LEU:HD12	0.41	1.93
1:A:42:PHE:HA	1:A:45:GLU:HG2	0.41	1.92
1:A:125:LEU:O	1:A:129:ILE:HG22	0.41	2.16
1:A:81:THR:HG21	1:A:85:TYR:CG	0.41	2.49
1:A:47:VAL:O	1:A:51:THR:N	0.41	2.53
1:A:47:VAL:HG23	1:A:78:VAL:HG21	0.41	1.92
1:A:22:VAL:CG2	1:A:129:ILE:HG21	0.40	2.46
1:A:134:ASP:HB2	1:A:137:GLN:OE1	0.40	2.16
1:A:101:TYR:O	1:A:105:HIS:CD2	0.40	2.74
1:A:28:PHE:CD1	1:A:36:VAL:HG21	0.40	2.52
1:A:6:ILE:CG2	1:A:125:LEU:HD12	0.40	2.45
1:A:97:ILE:CG1	1:A:122:MET:HE1	0.40	2.47
1:A:100:GLU:CB	1:A:122:MET:HE3	0.40	2.43

## 6.3 Torsion angles ⓘ

### 6.3.1 Protein backbone ⓘ

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all NMR entries. The Analysed column shows the number of residues for which the backbone conformation was analysed and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	138/140 (99%)	111 (80%)	21 (15%)	6 (4%)	6	30
All	All	138/140 (99%)	111 (80%)	21 (15%)	6 (4%)	6	30

All 6 Ramachandran outliers are listed below. They are sorted by the frequency of occurrence in the ensemble.

Mol	Chain	Res	Type
1	A	53	ALA
1	A	113	VAL
1	A	106	PRO
1	A	134	ASP
1	A	112	ASP
1	A	63	ASN

### 6.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all NMR entries. The Analysed column shows the number of residues for which the sidechain conformation was analysed and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	118/118 (100%)	77 (65%)	41 (35%)	1	10
All	All	118/118 (100%)	77 (65%)	41 (35%)	1	10

All 41 residues with a non-rotameric sidechain are listed below. They are sorted by the frequency of occurrence in the ensemble.

Mol	Chain	Res	Type
1	A	10	ARG
1	A	75	ILE
1	A	125	LEU
1	A	122	MET
1	A	121	LYS
1	A	131	LYS
1	A	55	GLU
1	A	80	ILE
1	A	15	LYS
1	A	9	PHE
1	A	116	THR
1	A	115	GLU
1	A	129	ILE

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Mol	Chain	Res	Type
1	A	43	PHE
1	A	79	LEU
1	A	105	HIS
1	A	6	ILE
1	A	134	ASP
1	A	109	GLU
1	A	28	PHE
1	A	117	ASN
1	A	11	SER
1	A	85	TYR
1	A	8	VAL
1	A	110	TRP
1	A	61	GLU
1	A	24	ASP
1	A	107	LYS
1	A	94	LEU
1	A	39	PHE
1	A	41	THR
1	A	124	GLN
1	A	98	LEU
1	A	102	LEU
1	A	23	LYS
1	A	59	ILE
1	A	83	LYS
1	A	113	VAL
1	A	47	VAL
1	A	71	ARG
1	A	91	TYR

### 6.3.3 RNA ⓘ

There are no RNA molecules in this entry.

### 6.4 Non-standard residues in protein, DNA, RNA chains ⓘ

There are no non-standard protein/DNA/RNA residues in this entry.

### 6.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 6.6 Ligand geometry

There are no ligands in this entry.

## 6.7 Other polymers

There are no such molecules in this entry.

## 6.8 Polymer linkage issues

There are no chain breaks in this entry.

## 7 Chemical shift validation

No chemical shift data were provided